

Generalized DMPK equation for strongly localized regime - numerical solution

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Generalized Dorokhov-Mello-Pereyra-Kumar (GDMPK) equation [K. A. Muttalib and J. R. Klauder, Phys. Rev. Lett. **82**, 4272 (1999)] has been proposed for the description of the electron transport in strongly localized systems. We develop an algorithm for the numerical solution of this equation and confirm that GDMPK equation correctly describes the critical and localized regimes. Contrary to the original DMPK equation, the generalized one contains also an information about the dimension of the system. In particular, it distinguishes between the two and the three dimensional models with the same number of transmission channels.

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Two decades ago, there was the belief that the distribution of the logarithm of the conductance, $\ln g$, of the strongly disordered electron system is Gaussian, independently on the dimension of the system. This paradigm was based on the two-terminal expression for the conductance,[1]

$$g = \frac{e^2}{h} \text{Tr } t^\dagger t = \sum_{i=1}^N \frac{1}{\cosh^2 x_i}. \quad (1)$$

Eq. (1) expresses the conductance in terms of parameters x_i which determine the eigenvalues of the matrix $t^\dagger t$ (t is the $N \times N$ transmission matrix and N is the number of open channels). Since all parameters x_i should increase linearly with the system size, $x_i \propto L$, it is natural to expect that in the limit of large L , only the contribution of the first channel (that one with the smallest parameter x) survives and $\ln g \approx -x_1 + \ln 4$. In the analogy with the one-dimensional (1D) case ($N = 1$), the distribution $p(\ln g)$ should be Gaussian. This is consistent with the solution of the Dorokhov-Mello-Pereyra-Kumar (DMPK) equation, [2] for very long quasi-one dimensional (Q1D) *weakly disordered* systems. [3]

However, numerical data [4] for *strongly disordered* 3D samples showed that $p(\ln g)$ is *not* Gaussian. Although all $x_i \propto L$, the mean values of the differences $x_{i+1} - x_i$, $i = 1, 2, \dots$ are constant, independent on the size of the system. Therefore, higher parameters, x_2, x_3, \dots , affect the form of the distribution $p(\ln g)$ in 3D. Since the deviation from Gaussian distribution cannot be obtained from the DMPK equation, the generalization of the last has been proposed by Muttalib and co-workers. [5, 6]

The derivation the DMPK equation[2] is based on the parametrization of the transfer matrix \mathbf{T} . For spin-less electrons and the time reversal symmetry of the system,

$$\mathbf{T} = \begin{pmatrix} u & 0 \\ 0 & u^* \end{pmatrix} \begin{pmatrix} \sqrt{1+\lambda} & \sqrt{\lambda} \\ \sqrt{\lambda} & \sqrt{1+\lambda} \end{pmatrix} \begin{pmatrix} v & 0 \\ 0 & v^* \end{pmatrix}, \quad (2)$$

where λ is a diagonal matrix with diagonal elements $\lambda_i = (1 + \cosh 2x_i)/2$, and u, v are unitary matrices.

[7] For sufficiently long systems, it is assumed that the elements of matrices u, v and λ are statistically independent. Contrary to the classical DMPK, the generalized DMPK equation (GDMPK) [5] contains additional $N(N-1)$ parameters,

$$K_{ij} = \left\langle \sum_{a=1}^N |u_{ia}|^2 |u_{ja}|^2 \right\rangle, \quad (3)$$

where $\langle \dots \rangle$ means a mean value over the realization of the disorder. The GDMPK equation reads

$$\ell \frac{\partial}{\partial L} P(\{x\}) = \frac{1}{4} \sum_{i=1}^N \frac{\partial}{\partial x_i} K_{ii} \left(\frac{\partial P}{\partial x_i} + P \frac{\partial}{\partial x_i} \Omega(\{x_n\}) \right). \quad (4)$$

Here, $P(\{x\})$ is the common probability distribution of all parameters x , ℓ is the mean free path, ℓ . The interaction potential $\Omega(\{x\})$ reads

$$\begin{aligned} \Omega(\{x_n\}) = & - \sum_{i < j} \gamma_{ji} \ln |\sinh^2(x_j) - \sinh^2(x_i)| \\ & - \sum_{i=1}^N \ln |\sinh(2x_i)|, \end{aligned} \quad (5)$$

and $\gamma_{ij} = 2K_{ij}/K_{ii}$,

Parameters K_{ij} depend on the strength of the disorder. For weak disorder, $K_{ij} = [1 + \delta_{ij}]/(N+1)$, $\gamma_{ij} \equiv 1$ and the GDMPK equation reduces to the classical DMPK equation. [2, 8] For general disorder we expect that K contains an information about the strength of the disorder, the topology and the dimensionality of the disordered system [10]. For instance, [5] $K_{11} \sim 1$ and $K_{12} \sim 1/L$ in the localized 3D regime. We expect that the transition from the metallic the insulating regime is associated with (continuous) change of parameters K [9, 10]. and the GDMPK equation with correct choice of parameters K describes the transport in the metallic, insulating and even in the critical regime. Note, the classical DMPK equation is not applicable to strongly disordered systems and contains no information about the dimension.

In Refs. [9, 10], a simplified GDMPK equation was introduced, with only two parameters: the diagonal elements $K_{ii} \equiv K_{11}$ for all i , and the off-diagonal elements

$K_{ij} \equiv K_{12}$ for all $i \neq j$. [11] An approximate solutions of such GDMPK equation, based on the saddle-point method [12] was obtained in Refs. [9, 10], and the solution was compared with numerical data obtained by the transfer matrix method (TM). Although quite satisfactory, agreement between approximate solutions and numerical data was obtained, a quantitative analysis of the solution of the GDMPK equation is still missing. Contrary to the DMPK equation, which is exactly solvable [13], no exact solution of the GDMPK equation is known. It is therefore highly desirable to solve the GDMPK equation numerically.

In this paper, we present an algorithm for the numerical solution of the GDMPK equation. Our method is based on the mapping of the GDMPK equation onto the Langevin equation, which describes the diffusion of N particles interacting with potential $\Omega(\{x\})$, given by Eq. (5). Simulating such diffusion, we obtain numerical solution of classical DMPK equation and the GDMPK equation. These solutions are compared with the numerical TM data for the tight-binding Anderson model,

$$\mathcal{H} = W \sum_r \varepsilon_r c_r^\dagger c_r + t_{\parallel} \sum_z c_r^\dagger c_{r'} + t_{\perp} \sum c_r^\dagger c_{r'} \quad (6)$$

which describes the transport of a single electron on the d -dimensional lattice. Random energies ε_r have zero mean value and variance $1/12$, W measures the strength of the disorder. Hopping term between two nearest neighboring sites r and r' is $t_{\parallel} = 1$ in the direction of the propagation and $t_{\perp} = 0.4$ in the perpendicular directions. For this choice of parameters, there are no evanescent (closed) channels in 2D and 3D systems. [14] In 3D, model (6) exhibits the disorder induced transition from the metal to the insulator at the critical point $W_c \approx 9.2$. [10, 15]

Our numerical method uses the fact that the GDMPK equation (4) is a special Fokker-Planck diffusion equation

$$\frac{\partial}{\partial s} P = \left(-\frac{\partial}{\partial x_i} D_i^{(1)}(\{x\}) + \frac{\partial^2}{\partial x_i^2} D_i^{(2)}(\{x\}) \right) P \quad (7)$$

for the one dimensional diffusion of N particles located at x in “time” $s = L/\ell$. The common probability distribution $P(\{x\}, s)$ determines the positions of all particles at time s . In Eq. (7), $D_i^{(1)}$ and $D_i^{(2)}$ are the drift and the diffusion coefficients. The Fokker Planck equation (7) describes the random process given by the Langevin equation, [16]

$$\partial x_i / \partial s = h_i(\{x\}, s) + g_i(\{x\}) \Gamma_i(s), \quad (8)$$

with random white noise force $\Gamma(s)$, $\langle \Gamma(s) \rangle = 0$ and $\langle \Gamma(s) \Gamma(s') \rangle = 2\delta(s - s')$, and coefficients

$$h_i = D_i^{(1)} - \sqrt{D_i^{(2)}} \frac{\partial}{\partial x_i} \sqrt{D_i^{(2)}} \quad \text{and} \quad g_i = \sqrt{D_i^{(2)}}. \quad (9)$$

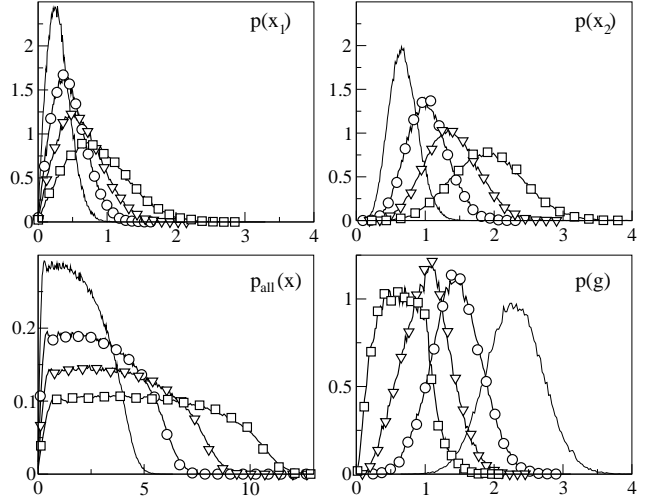


FIG. 1: The test of the numerical algorithm. The classical DMPK equation is solved for $N = 9$ channels. Results are compared with the TM data for the Anderson model on the lattice $3 \times 3 \times L$ and disorder $W = 2$. Solid lines are the TM data for $L = 30$ (used as initial condition for the DMPK equation), and $L = 50, 70$, and 100 . Symbols show solutions of the DMPK equation for $s = 1.8$ (circles), 3.6 (triangles) and 6.35 (squares). For these parameters, both the TM and the DMPK solutions have the same value of the mean conductance $\langle g \rangle$.

Comparison of Eqs. (4) with Eq. (7) gives

$$D_i^{(1)} = -\frac{K_{ii}}{4} \frac{\partial \Omega(\{x_n\})}{\partial x_i}, \quad \text{and} \quad D_i^{(2)} = \frac{K_{ii}}{4}. \quad (10)$$

We simulate the Langevin force Γ , integrate the equation of motion (8) and take the average for a large number of realizations. The numerical integration of the equation (8) gives

$$x_{i(n+1)} = x_{in} + D_i^{(1)}(\{x\})\delta s + \sum_{j=1}^N \sqrt{D_i^{(2)}(\{x\})\delta s} \times w_{in}, \quad (11)$$

where N is the number of particles and δs is the “time” step. Statistically independent Gaussian variables w_{in} have zero mean and variance $\langle w_{jn} w_{kn'} \rangle = 2\delta_{jk}\delta_{nn'}$. After n integration steps we obtain the stochastic variables $x_{in} = x_i(s)$ at “time” $s = n \times \delta s$.

In simulations, we have to keep the ordering, $x_1 < x_2 < \dots < x_N$. Therefore, the position of the i th particle is restricted as $x_{i-1n} < x_{in} < x_{i+1n-1}$. To keep this constrain, the “time” step, δs must be very small. For x_{1n} the left boundary is 0. To avoid numerical overflows, we introduce and we use the “cutoff” C , $x_{Nn} \leq C, \forall n$.

We are not able to start the numerical algorithm with the ballistic initial values, $\lim_{L \rightarrow 0} P = \prod_i \delta(\lambda_i - 0^+)$, used in the formulation of the DMPK equation. To avoid this difficulty, we use the TM method and calculate first the distributions $p(x_i)$ for the Anderson model for a short

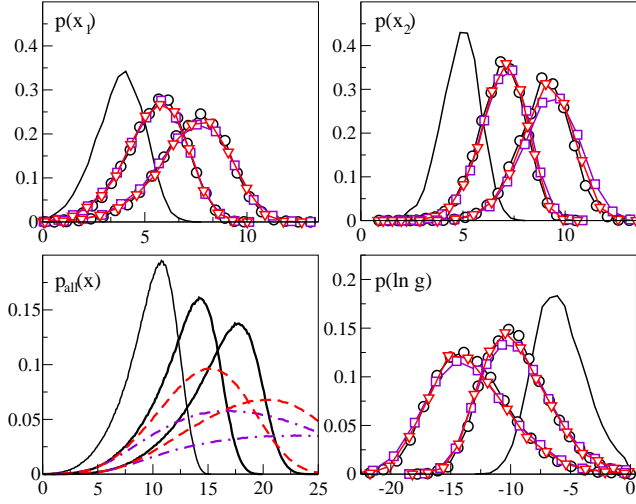


FIG. 2: (Color online) The 3D Anderson model $7 \times 7 \times L$ with disorder $W = 29$ (strongly localized regime). Solid line shows the TM data for $L = 6$, circles are the TM data for lengths $L = 8$ and $L = 10$, which are compared with the GDMPK data for $s = 10.5$ and 20 , respectively. In the GDMPK equation, we use either entire matrix K_{ij} (triangles) or the two-parameter model (squares) with $K_{11} = 0.5225$ and $K_{12} = 0.0244$. Estimated mean free path $\ell \approx 0.2$ is consistent with [10]. The GDMPK data for $p_{\text{all}}(x)$ are shown by dashed and dot-dashed lines for model with complete matrix K and the model with K_{11} and K_{12} , respectively.

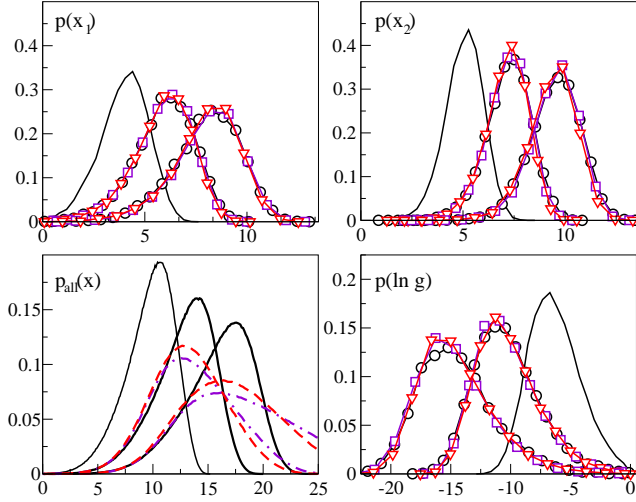


FIG. 3: (Color online) The 2D Anderson model $49 \times L$ and $W = 26$. Initial condition are given by the TM data for $L = 6$ (solid line). The TM data for $L = 8$ and $L = 10$ are compared with the GDMPK data for $N = 49$ channels and $s = 9.5$ and 19 ($\ell \approx 0.21$). The symbols have the same meaning as in Fig. 2. We used $K_{11} = 0.712$ and $K_{12} = 0.0837$ in the two parameter GDMPK equation.

length L_0 of the system. We use these distribution as initial values for the GDMPK equation. The TM data for $L = L_0$ provides us also with the values of parameters K . The solution of the GDMPK equation is compared with

the TM result for length $L > L_0$. In the TM method, the length is defined as a number of lattice sites along the propagation direction. For a given L , we find the length s in the GDMPK equation from the condition that the mean conductance (or the mean of logarithm of the conductance in strongly localized regime) found by the two methods coincides. We find in this way also the mean free path (in units of the lattice period of the Anderson model): $\ell = (L - L_0)/s$.

Our results are summarized in Figs. 1-5. Compared are four distributions: $p(x_1)$ and $p(x_2)$ for the two smallest parameters x , the distribution $p_{\text{all}}(x)$ of all parameters x , $p_{\text{all}}(x) = \langle \sum_i^N \delta(x - x_i) \rangle$, and the distribution of the conductance $p(g)$ or of the logarithm of the conductance, $p(\ln g)$.

In order test the numerical algorithm, we solve first the classical DMPK equation. Fig. 1 shows the data for the weakly disordered Q1D systems with $N = 9$. The length of the system varies between $L = 30$ (initial condition for the DMPK) and $L = 100$. The “time” step used in the solution of the DMPK equation $\delta s = 10^{-4}$ and 63.500 iterations were performed. With the use of appropriate length s , we obtained perfect agreement between the DMPK and TM data, and also estimate the mean free path, $\ell \approx 11$, consistent with $\ell \approx 9.2$ estimated for the 3D anisotropic systems [10].

In Figs. 2 and 3 we present the solution of the GDMPK equation for $N = 49$ channels in the strongly disordered regime (disorder $W = 26$). In Fig. 2 we simulate the transport through the 3D system $7 \times 7 \times L$. The TM data for $L = 6$ provides us with the initial distributions for the GDMPK as well as with values of parameters K . Data for $L = 8$ and $L = 10$ are then compared with two solutions of the GDMPK: in the first simulations, we use the entire matrix K_{ij} , and in the second simulation, we substitute all diagonal elements by K_{11} and all off-diagonal terms by K_{12} . Fig. 3 summarizes the TM results for the transport through the 2D strongly disordered system $49 \times L$ ($W = 26$) compared with the corresponding solution of the GDMPK equation.

Both Figures show that the GDMPK data for $p(x_1)$, $p(x_2)$ and $p(\ln g)$ agree with results of the TM simulations. Since the TM data were obtained for systems of different dimension, we conclude that the GDMPK equations distinguishes between the 2D and 3D disordered systems. The information about dimension is given in parameters K_{11} and K_{12} .

The difference between the 2D and 3D systems is more clearly visible in Figs. 4 and 5 which compares 3D TM data for the critical disorder $W_c = 9.2$ and 2D data for $W = 8.6$. Although both system have approximately the same mean free path, the conductance distributions differ from each other when L increases.

Obtained results confirm that already the simplified two-parameter GDMPK equation determines correctly the statistics of the conductance, both in the localized

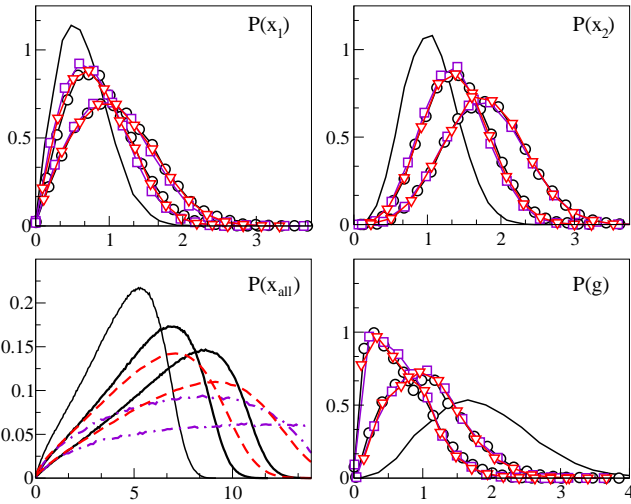


FIG. 4: (Color online) The 3D Anderson model $7 \times 7 \times L$ with critical disorder $W_c = 9.2$ Solid lines show the TM data for $L = 6$ (initial condition). The TM data for $L = 10$ are compared with the GDMPK data for $N = 49$ and length $s = 3.25$ and 6.375 ($\ell \approx 0.63$).

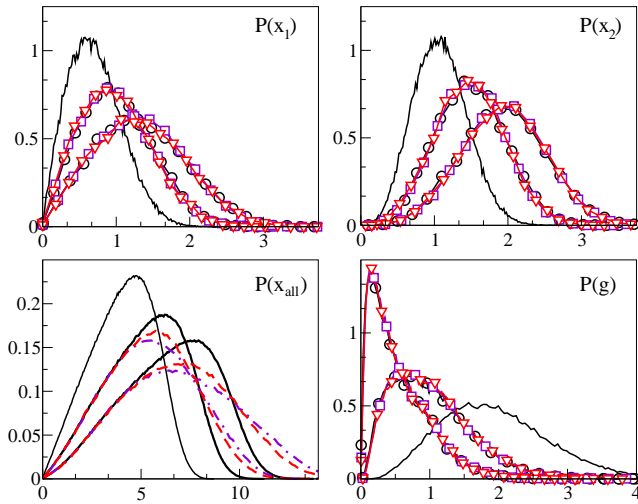


FIG. 5: (Color online) The 2D Anderson model $49 \times L$ with disorder $W = 8.6$ Solid lines: the TM data for $L = 6$ (Initial condition). Circles: the TM data for $L = 8$ and $L = 10$ compared with the GDMPK data for $s = 3.375$ and $s = 6.5$, respectively ($\ell \approx 0.615$). Symbols have the same meaning as in Fig. 2.

and critical regimes. However, the total distribution of all parameters x , $p_{\text{all}}(x)$, is reproduced only for rather small values of x . The possible reason for this discrepancy is that the TM data for the entire matrix K might not be sufficiently accurate for high indices i and j , so that we do not know true values of repulsion constants γ_{ij} for higher channels. In the two parameter model, K_{11} and K_{12} , might overestimate the repulsion of higher channels (for instance $\gamma_{1i} \sim i^{-1/2}$ [10]). This overestimation broads the distribution $p_{\text{all}}(x)$. Interestingly, the 2D

data for $p_{\text{all}}(x)$ are more accurate than the data for 3D. Nevertheless, as argued previously [17], and confirmed by our data shown in Figs. 2-5, we do not need to know the distribution of all parameters x for the description of the statistics of the conductance. Only small portion of channels is important for the description of the critical regime in 3D.

In conclusion, we presented numerical solution of the generalized DMPK equation. Our results confirm that the generalized DMPK equation describes correctly the electron transport in the localized and the critical regime. The information about the dimension of the system is given by the additional parameters, K_{11} and K_{12} [11]. We hope that analytical solution of the generalized DMPK equation could provide us with the analytical description of the electron transport in the critical and localized regimes in various dimensions.

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